Generative Models for De Novo Drug Design.

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Abstract

Artificial intelligence (AI) is booming. Among various AI approaches, generative models have received much attention in recent years. Inspired by these successes, researchers are now applying generative model techniques to de novo drug design, which has been considered as the "holy grail" of drug discovery. In this Perspective, we first focus on describing models such as recurrent neural network, autoencoder, generative adversarial network, transformer, and hybrid models with reinforcement learning. Next, we summarize the applications of generative models to drug design, including generating various compounds to expand the compound library and designing compounds with specific properties, and we also list a few publicly available molecular design tools based on generative models which can be used directly to generate molecules. In addition, we also introduce current benchmarks and metrics frequently used for generative models. Finally, we discuss the challenges and prospects of using generative models to aid drug design.